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NATURE OF DONORS IN SiC*

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6H-SiC samples were examined by ESR technique in temperature range from 5 K up to 300 K. Two kinds of ESR lines were observed: a single line at $g = 2.0054 \pm 0.0007$, called X-line, and a triplet corresponding to isolated nitrogen defect. Ionization energy of X defect was determined as about 60 meV and the ionization energy of isolated nitrogen was determined as about 200 meV below SiC conduction band.

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1. Introduction

Isolated nitrogen placed at carbon site is a basic donor in SiC as identified by ESR. Its spectrum consists of three lines of equal amplitudes [1] due to hyperfine interaction of nuclear spin $I = 1$. On the other hand, ionization energies of shallow donors in SiC have been determined by IR absorption measurements as 60, 138 and 142 meV [2]. Up to now these three values have been typically connected with isolated nitrogen donors occupying three possible positions in 6H-SiC crystal lattice. However, absorption measurements did not allow to identify defects related to the observed bands and therefore there is still some doubts if isolated nitrogen centers are the only shallow donors in SiC.

The aim of this paper was to identify shallow donors in SiC crystals by use of ESR experiments and estimate their energy position from temperature dependence of ESR lines.

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2. Experiment

6H-SiC samples were grown at the Institute of Electronic Materials Technology in Warsaw using Lely method [3] and in the Institute of Semiconductors Physics in Kiev using Lely and Acheson method [4]. They were examined by ESR technique. X-band Bruker spectrometer was used, the samples were kept in continuous flow cryostat which allowed measurements with different microwave power in temperature range from 5 K up to 300 K. A typical spectrum of 6H-SiC sample measured at different temperatures is shown in Fig. 1. Two kinds of ESR lines were

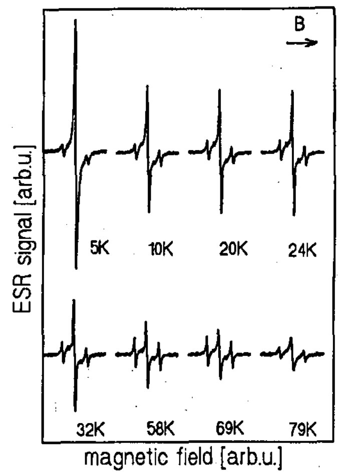

Fig. 1. ESR signal of typical n-type 6H-SiC crystal as a function of temperature.

observed: a single line at $g = 2.0054 \pm 0.0007$ (seen as a central line in Fig. 1) called X-line and a triplet consisting of three equally spaced lines with the middle one overlapping X-line. The relative intensities of the singlet and the triplet changed from sample to sample. Temperature dependencies of the singlet and the triplet intensities are presented in Fig. 2.

3. Discussion

Typical behavior of ESR line is its broadening with temperature increase and change of its amplitude as $1/T$. This is not the case for both observed defects in the presented paper. As seen from Fig. 2, line intensities multiplied by T are not constant functions of temperature. The increase in the signals with increasing temperature at low temperature region is due to ESR signal saturation, whereas decrease at high temperature should be first of all connected with defect ionization. Generally, when ESR amplitude decreases without a change of a line width (which is the case for both observed defects), one can suspect that corresponding defect is getting ionized. Therefore, temperature dependence of ESR line amplitude can be a way of estimating defect ionization energy as described below.

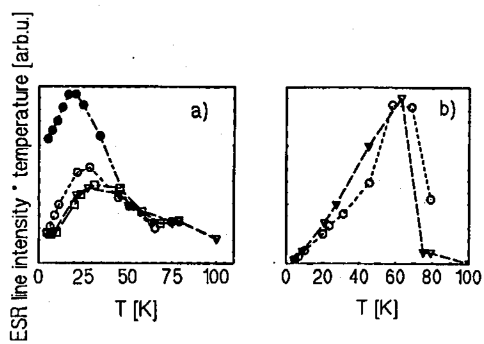

Fig. 2. **Temperature dependencies of ESR line intensities in SiC (multiply by temperature): (a) X-line, (b) one of triplet lines corresponding to isolated nitrogen.**

In thermal equilibrium concentration of electrons trapped on a single donor level is described as

$$n_\mathrm{d} = \frac{N_\mathrm{d}}{\frac{1}{2}\exp\left(\frac{E_\mathrm{d}-E_\mathrm{F}}{kT}\right)+1}, \tag{1}$$

where E_F is a Fermi level energy and N_d, E_d — concentration and energy of donors respectively. For low enough temperature Fermi level E_F is given by

$$E_\mathrm{F} = kT\ln\left\{\frac{1}{4}\left[\sqrt{1+\frac{8N_\mathrm{d}}{N_\mathrm{c}}\exp\left(\frac{E_\mathrm{d}}{kT}\right)}-1\right]\exp\left(\frac{E_\mathrm{d}}{kT}\right)\right\}, \tag{2}$$

where N_c is density of states in the conduction band.

As a result of the performed experiment quite different temperature dependencies of ESR X-line amplitude in comparison with ESR nitrogen triplet were obtained as is easily seen from Fig. 2. Temperature corresponding to decrease in curves related to X defect (a) was about 30–40 K whereas for nitrogen center (b) it was about 70–80 K. Taking into account defect ionization with temperature according to formula (1) two different ionization energies for both defects were estimated. This is the first estimation of ionization energies and fittings to experimental points are not sufficiently good, yet. However, they allow to describe the departure of experimental points from $1/T$ dependence (Fig. 3). Further calculations are in progress.

For the defect attributed to X-line the ionization temperature was about 30 K. In one of the measured samples X defect concentration was estimated as about 10^{18} cm^{-3} (from ESR line intensity). Taking into account this number, the ionization energy of X defect was obtained as about 60 meV.

For isolated nitrogen the ionization temperature was about 70 K. In two of the measured samples the concentration of nitrogen was estimated as about 10^{16} cm^{-3}. Taking into account this number, the ionization energy of isolated nitrogen was obtained as about 200 meV.

Fittings to the experimental curves using formula (1) are presented in Fig. 3. They allowed to estimate ionization energies of both donors.

In summary it was possible to attribute 60 meV donor to X defect and 200 meV to isolated nitrogen center. The still open question is a nature of X

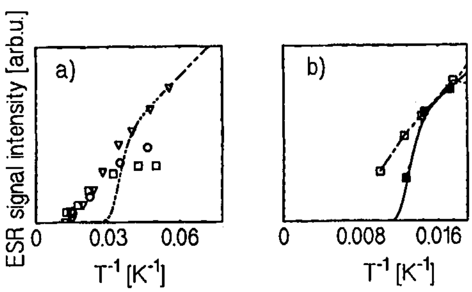

Fig. 3. Temperature dependencies of ESR line intensities in SiC (point) together with calculated curves obtained using formula (1) for (a) X-line, (b) isolated nitrogen lines.

defect. Its nuclear spin should be $I = 0$. The possible candidate is a vacancy defect.

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